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Enthalpy of solvation correlations for organic solutes and gases dissolved in dichloromethane and 1,4-dioxane

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Abstract

Enthalpies of solution at infinite dilution of 53 organic solutes in dichloromethane and 10 organic solutes in 1,4-dioxane were measured using semi-adiabatic solution calorimeter. Enthalpies of solvation for 103 organic vapors and gaseous solutes in dichloromethane and for 116 gaseous compounds in 1,4-dioxane were determined from the experimental and literature data. It is shown that an Abraham solvation equation with five descriptors can be used to correlate the experimental solvation enthalpies within standard deviations of 2.07 and 2.29 kJ mol-1 for dichloromethane and 1,4-dioxane, respectively. The derived correlations provide very accurate mathematical descriptions of the measured enthalpy of solvation data at 298 K, which in the case of 1,4-dioxane span a range of 121 kJ mol-1. Division of the experimental values into a training set and a test set shows that there is no bias in predictions, and that the predictive capability of the correlations is better than 3.5 kJ mol-1. Enthalpies of hydrogen bond formation of proton donor solutes (alcohols, amines, chlorinated hydrocarbons, etc.) with 1,4-dioxane were calculated based on the Abraham solvation equation. Obtained values are in good agreement with the available literature data. © 2013 Springer Science+Business Media New York.

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Keywords

Enthalpy of hydrogen bond, Enthalpy of solution, Enthalpy of solvation, Enthalpy of transfer, Mathematical correlation, Solvation parameter model